



wwPDB EM Validation Summary Report ⓘ

Nov 2, 2024 – 07:27 pm GMT

PDB ID : 6RAX
EMDB ID : EMD-4786
Title : D. melanogaster CMG-DNA, State 1B
Authors : Eickhoff, P.; Martino, F.; Costa, A.
Deposited on : 2019-04-08
Resolution : 3.99 Å(reported)

This is a wwPDB EM Validation Summary Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

EMDB validation analysis	:	0.0.1.dev113
Mogul	:	1.8.4, CSD as541be (2020)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.39

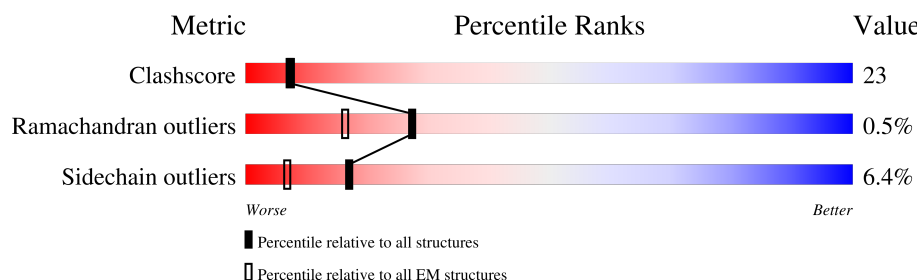
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.99 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	210492	15764
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion $< 40\%$). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	2	887	
2	3	819	
3	4	866	
4	5	733	
5	6	817	
6	7	720	
7	X	21	
8	Y	8	

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Mol	Chain	Length	Quality of chain
9	A	575	
10	H	202	
11	L	203	
12	M	212	
13	N	228	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
14	ATP	3	901	-	-	X	-

2 Entry composition

There are 15 unique types of molecules in this entry. The entry contains 40970 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called DNA replication licensing factor Mcm2.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	2	605	Total	C	N	O	S	0	0
			4788	3023	835	899	31		

- Molecule 2 is a protein called DNA replication licensing factor Mcm3.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	3	625	Total	C	N	O	S	0	0
			4879	3044	868	939	28		

- Molecule 3 is a protein called DNA replication licensing factor MCM4.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	4	626	Total	C	N	O	S	0	0
			5013	3150	886	951	26		

- Molecule 4 is a protein called DNA replication licensing factor Mcm5.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	5	620	Total	C	N	O	S	0	0
			4864	3047	869	917	31		

- Molecule 5 is a protein called DNA replication licensing factor Mcm6.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	6	628	Total	C	N	O	S	0	0
			4986	3121	882	954	29		

- Molecule 6 is a protein called DNA replication licensing factor Mcm7.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	7	636	Total	C	N	O	S	0	1
			4964	3100	885	945	34		

- Molecule 7 is a DNA chain called DNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	X	21	Total	C	N	O	P	0	0
			424	208	56	139	21		

- Molecule 8 is a DNA chain called DNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	Y	8	Total	C	N	O	P	0	0
			164	78	30	48	8		

- Molecule 9 is a protein called CDC45L.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	A	567	Total	C	N	O	S	0	0
			4575	2900	791	862	22		

- Molecule 10 is a protein called IP07275p.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	H	195	Total	C	N	O	S	0	0
			1583	1007	279	289	8		

- Molecule 11 is a protein called Probable DNA replication complex GINS protein PSF2.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	L	185	Total	C	N	O	S	0	0
			1498	962	252	271	13		

- Molecule 12 is a protein called AT18545p.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	M	167	Total	C	N	O	S	0	0
			1381	877	245	255	4		

- Molecule 13 is a protein called DNA replication complex GINS protein SLD5.

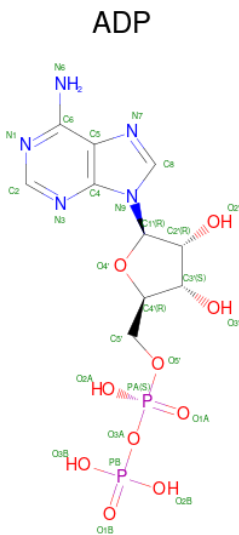
Mol	Chain	Residues	Atoms					AltConf	Trace
13	N	208	Total	C	N	O	S	0	0
			1677	1042	285	337	13		

- Molecule 14 is ADENOSINE-5'-TRIPHOSPHATE (three-letter code: ATP) (formula: C₁₀H₁₆N₅O₁₃P₃) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					AltConf
14	2	1	Total 31	C 10	N 5	O 13	P 3	0
14	3	1	Total 31	C 10	N 5	O 13	P 3	0
14	5	1	Total 31	C 10	N 5	O 13	P 3	0

- Molecule 15 is ADENOSINE-5'-DIPHOSPHATE (three-letter code: ADP) (formula: $\text{C}_{10}\text{H}_{15}\text{N}_5\text{O}_{10}\text{P}_2$) (labeled as "Ligand of Interest" by depositor).

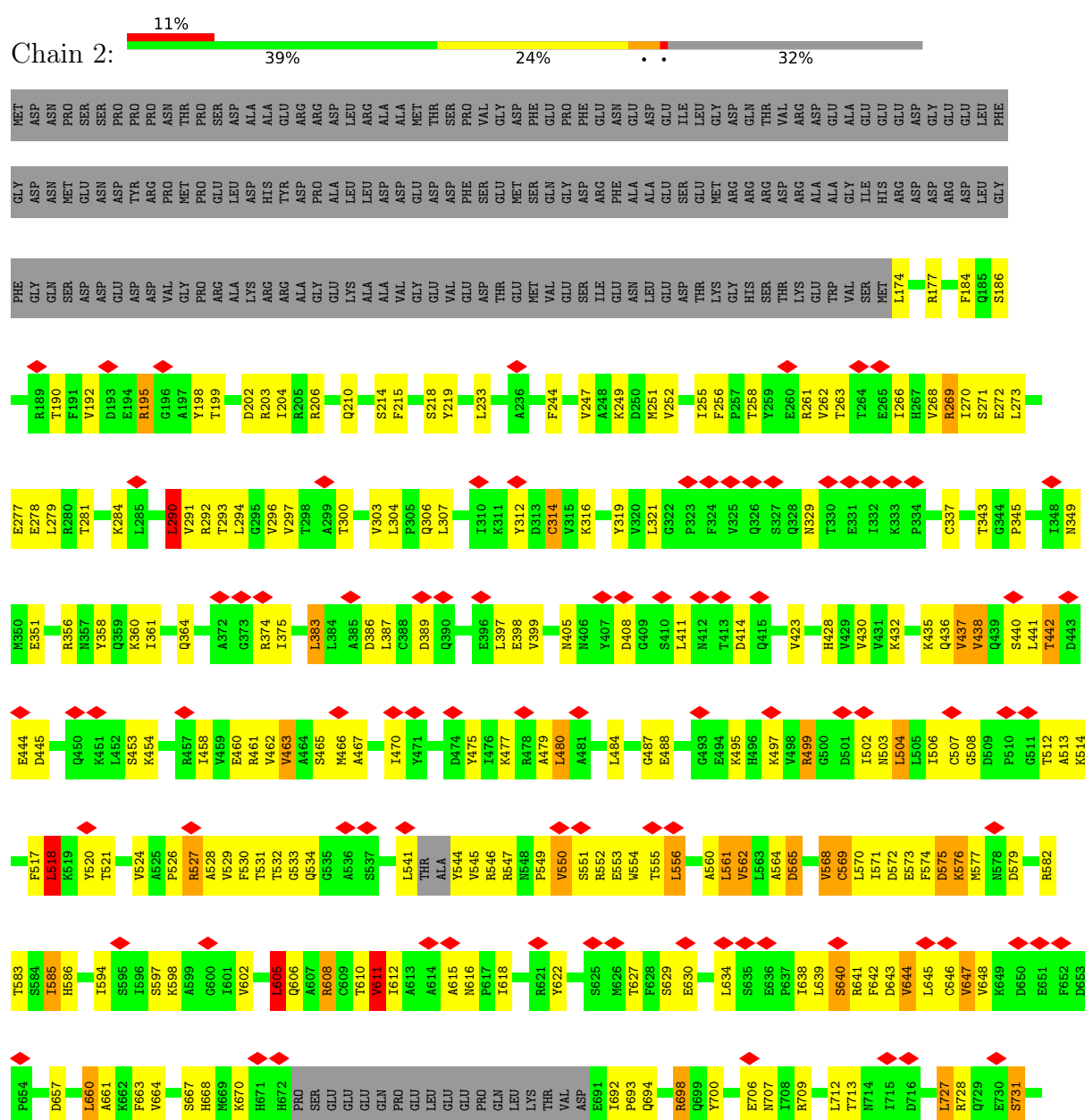


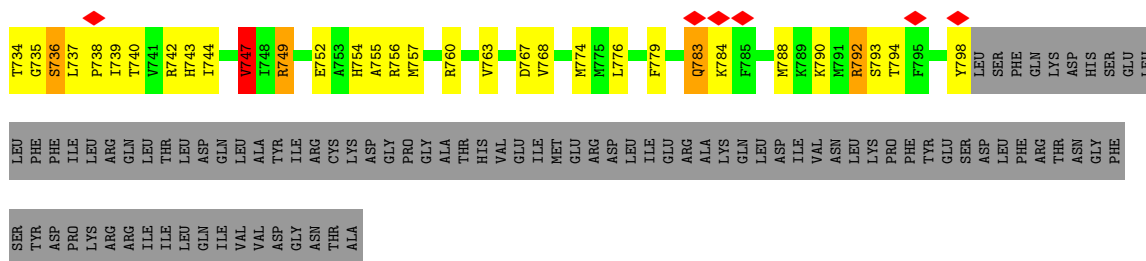
Mol	Chain	Residues	Atoms					AltConf
15	4	1	Total	C	N	O	P	0
			27	10	5	10	2	
15	6	1	Total	C	N	O	P	0
			27	10	5	10	2	
15	7	1	Total	C	N	O	P	0
			27	10	5	10	2	

3 Residue-property plots

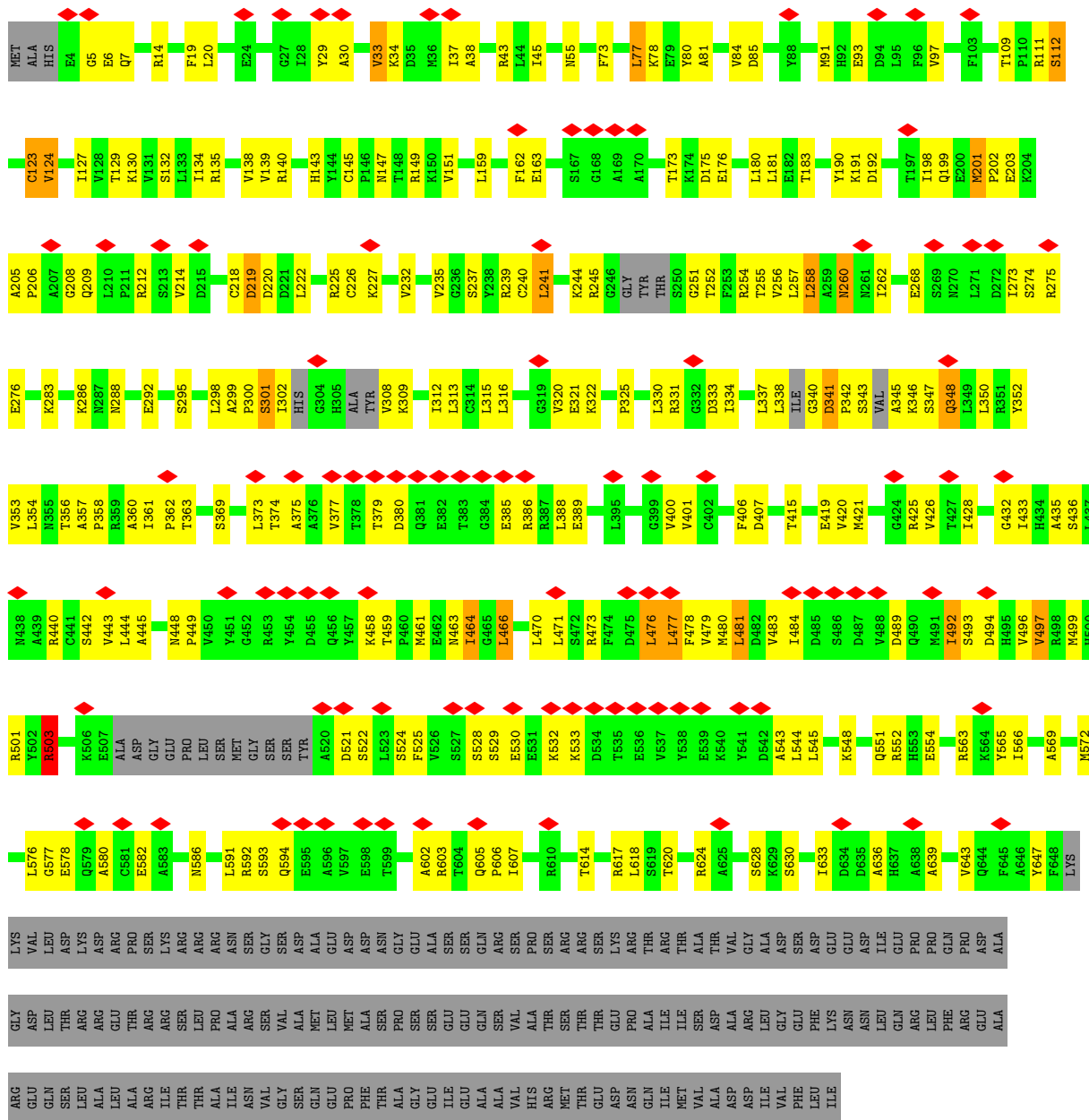
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion in map density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

- Molecule 1: DNA replication licensing factor Mcm2

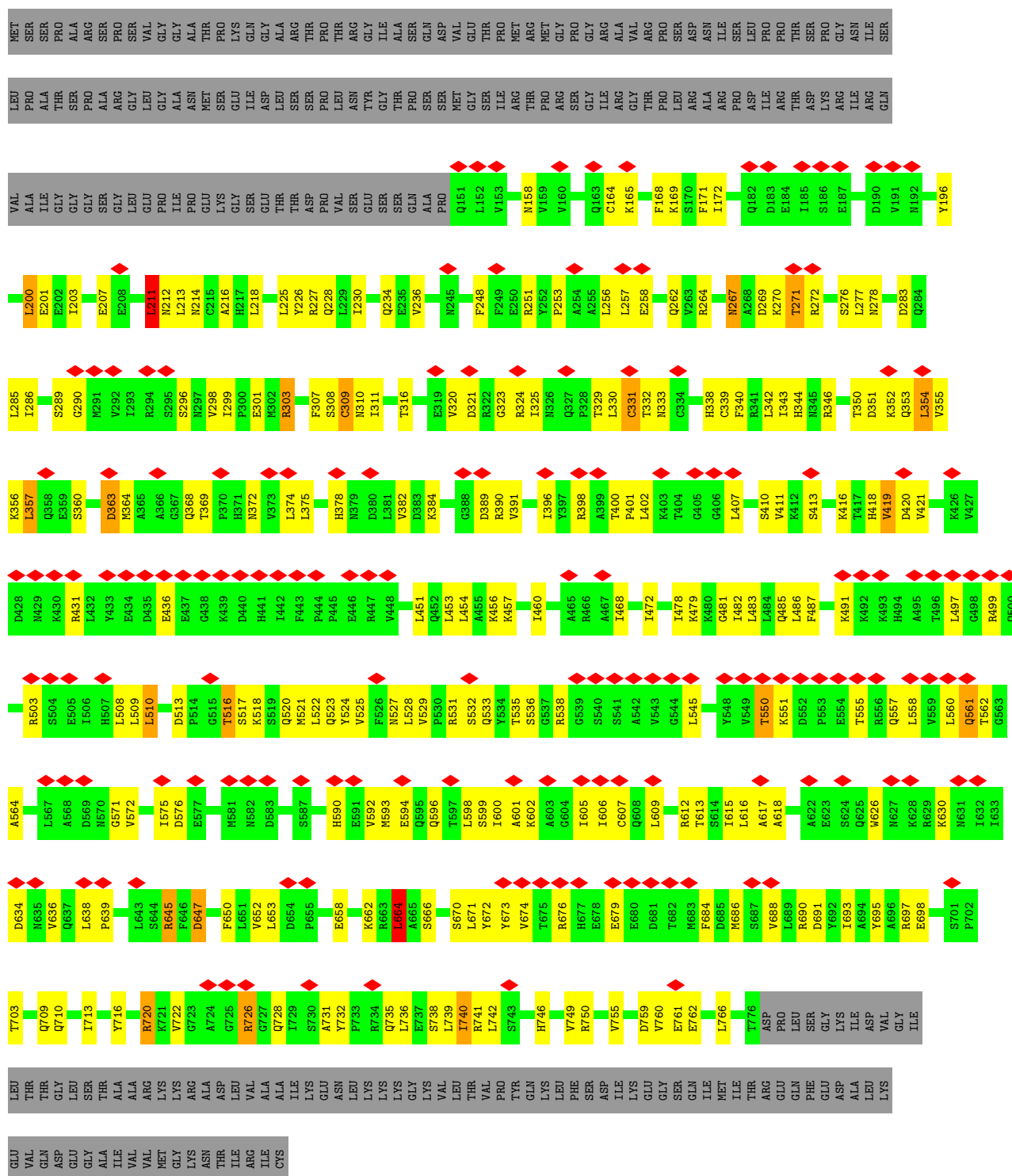
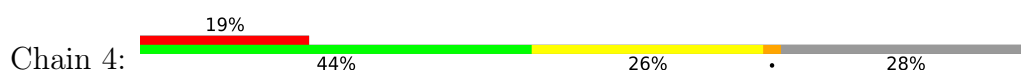




• Molecule 2: DNA replication licensing factor Mcm3

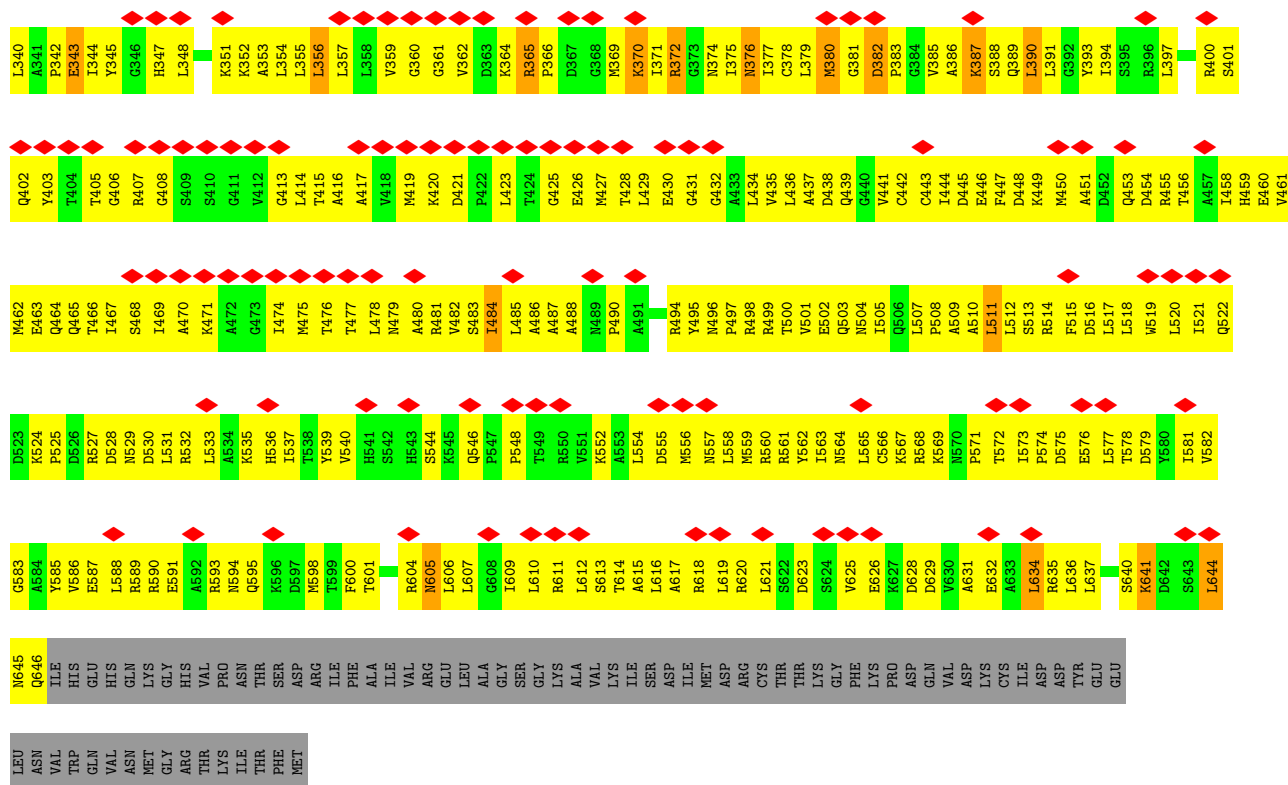


• Molecule 3: DNA replication licensing factor MCM4



- Molecule 4: DNA replication licensing factor Mcm5





• Molecule 7: DNA

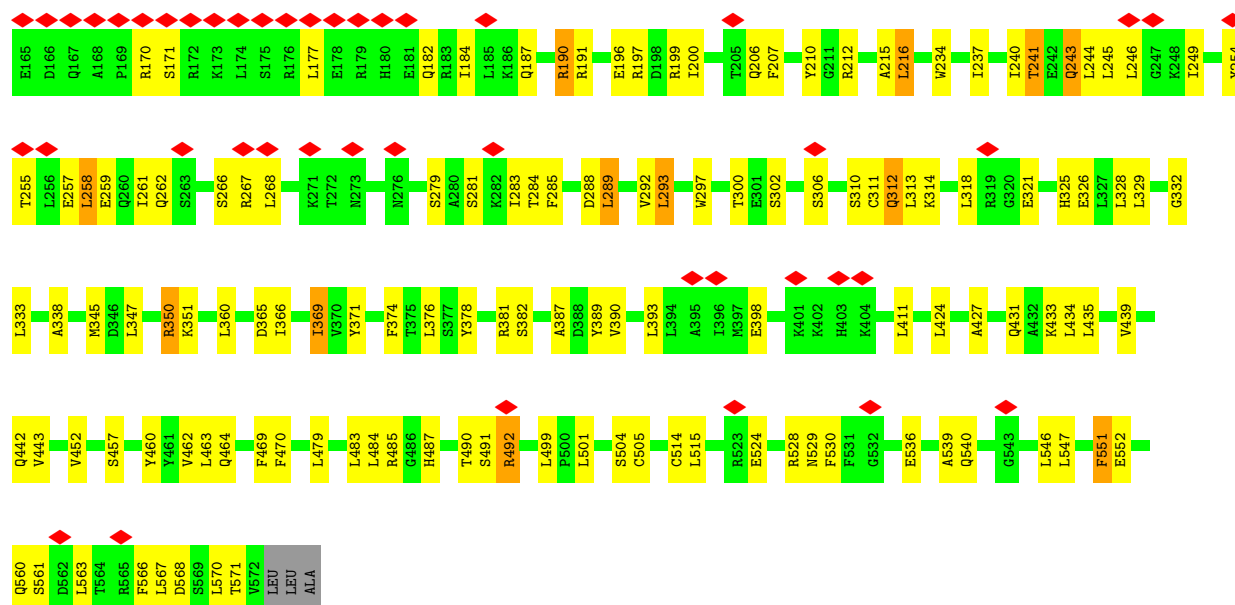


• Molecule 8: DNA

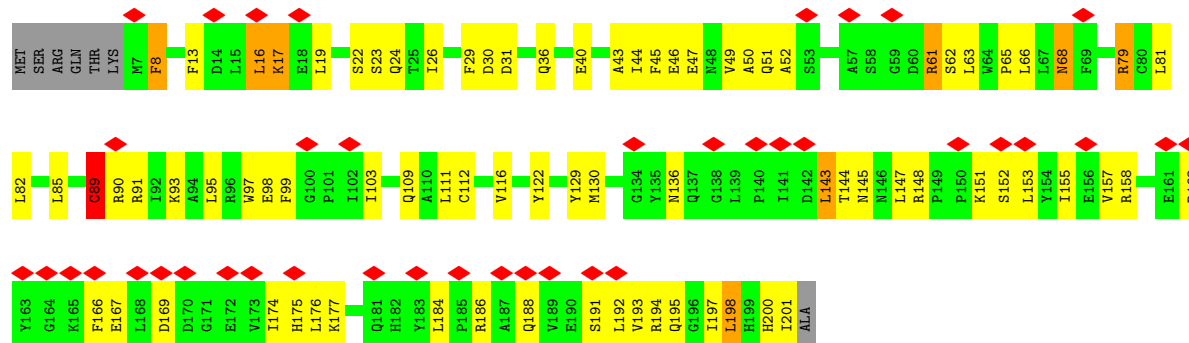


• Molecule 9: CDC45L

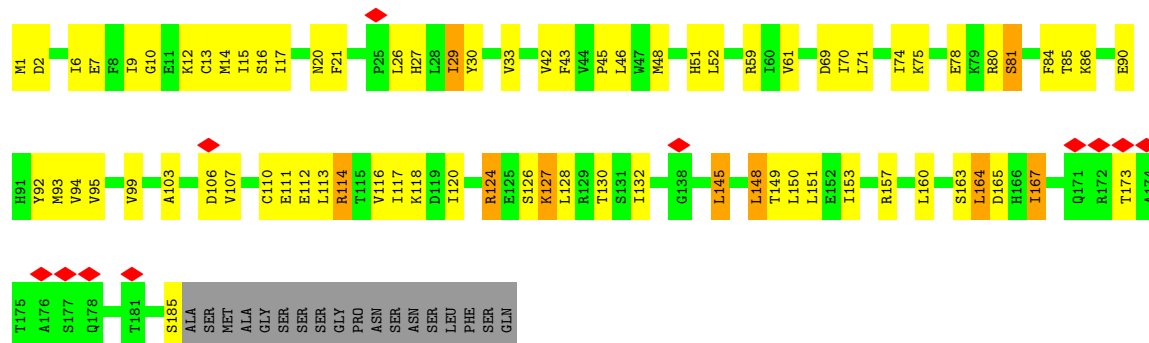




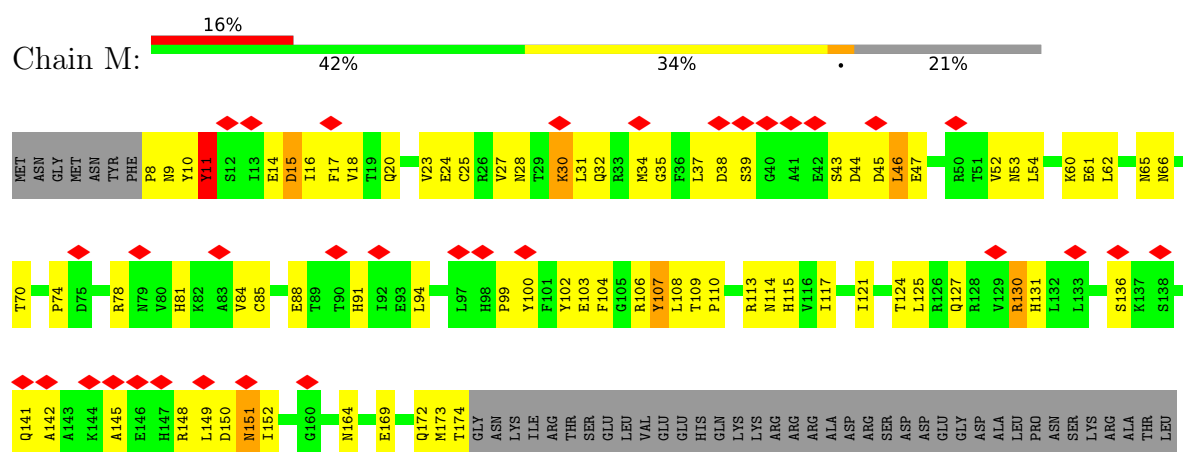
• Molecule 10: IP07275p



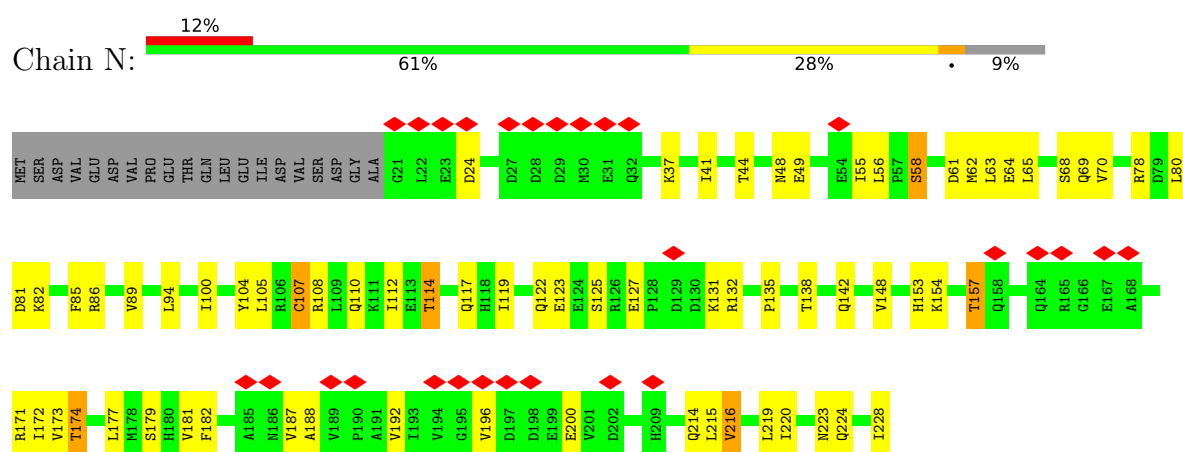
• Molecule 11: Probable DNA replication complex GINS protein PSF2



• Molecule 12: AT18545p



• Molecule 13: DNA replication complex GINS protein SLD5



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	92754	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	50	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.066	Depositor
Minimum map value	-0.047	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.001	Depositor
Recommended contour level	0.006	Depositor
Map size (Å)	414.72003, 414.72003, 414.72003	wwPDB
Map dimensions	384, 384, 384	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.08, 1.08, 1.08	Depositor

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: ATP, ADP

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# $ Z > 5$	RMSZ	# $ Z > 5$
1	2	0.53	0/4874	1.00	32/6587 (0.5%)
2	3	0.51	1/4946 (0.0%)	0.85	13/6664 (0.2%)
3	4	0.44	0/5106	0.75	2/6912 (0.0%)
4	5	0.58	0/4939	0.85	11/6646 (0.2%)
5	6	0.49	1/5064 (0.0%)	0.82	9/6834 (0.1%)
6	7	0.36	0/5029	0.66	0/6775
7	X	0.81	0/469	1.47	5/722 (0.7%)
8	Y	0.60	0/183	1.04	0/280
9	A	0.58	1/4669 (0.0%)	0.82	5/6312 (0.1%)
10	H	0.61	1/1618 (0.1%)	0.85	2/2184 (0.1%)
11	L	0.65	0/1534	0.84	2/2076 (0.1%)
12	M	0.71	1/1413 (0.1%)	0.87	3/1914 (0.2%)
13	N	0.55	0/1703	0.78	0/2304
All	All	0.53	5/41547 (0.0%)	0.84	84/56210 (0.1%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	2	1	4
2	3	0	4
3	4	0	9
4	5	0	11
5	6	0	5
6	7	0	1
9	A	0	3
10	H	0	2
11	L	0	2
12	M	0	8

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Mol	Chain	#Chirality outliers	#Planarity outliers
13	N	0	2
All	All	1	51

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	M	11	TYR	CD1-CE1	-7.23	1.28	1.39
10	H	89	CYS	CB-SG	-5.25	1.73	1.81
5	6	454	PHE	CD1-CE1	-5.11	1.29	1.39
9	A	297	TRP	CB-CG	-5.10	1.41	1.50
2	3	503	ARG	C-N	5.03	1.45	1.34

The worst 5 of 84 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	6	521	ARG	NE-CZ-NH2	-16.89	111.86	120.30
1	2	499	ARG	C-N-CA	11.83	147.14	122.30
1	2	466	MET	C-N-CA	11.03	149.28	121.70
1	2	518	LEU	CB-CG-CD1	10.78	129.33	111.00
7	X	0	DG	O4'-C1'-C2'	-10.69	97.35	105.90

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	2	585	ILE	CB

5 of 51 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	2	437	VAL	Peptide
1	2	497	LYS	Peptide
1	2	527	ARG	Peptide
1	2	569	CYS	Peptide
2	3	201	MET	Peptide

5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	2	4788	0	4825	187	0
2	3	4879	0	4914	196	0
3	4	5013	0	4999	174	0
4	5	4864	0	4911	216	0
5	6	4986	0	4983	156	0
6	7	4964	0	4992	642	0
7	X	424	0	247	43	0
8	Y	164	0	91	6	0
9	A	4575	0	4493	136	0
10	H	1583	0	1567	61	0
11	L	1498	0	1519	61	0
12	M	1381	0	1352	55	0
13	N	1677	0	1623	58	0
14	2	31	0	12	2	0
14	3	31	0	11	10	0
14	5	31	0	12	5	0
15	4	27	0	12	2	0
15	6	27	0	12	3	0
15	7	27	0	12	8	0
All	All	40970	0	40587	1883	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 23.

The worst 5 of 1883 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:7:237:MET:HB2	6:7:255:ILE:HD11	1.27	1.10
6:7:441:VAL:HG22	6:7:483:SER:HB2	1.37	1.06
4:5:589:ARG:HB2	4:5:607:ILE:HG21	1.39	1.00
6:7:336:LEU:HD11	6:7:559:MET:HG2	1.42	1.00
6:7:206:CYS:HB2	6:7:211:CYS:HB3	1.40	0.99

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	2	599/887 (68%)	445 (74%)	148 (25%)	6 (1%)	13	47
2	3	611/819 (75%)	492 (80%)	116 (19%)	3 (0%)	25	61
3	4	624/866 (72%)	520 (83%)	101 (16%)	3 (0%)	25	61
4	5	608/733 (83%)	471 (78%)	134 (22%)	3 (0%)	25	61
5	6	624/817 (76%)	511 (82%)	111 (18%)	2 (0%)	37	71
6	7	623/720 (86%)	537 (86%)	85 (14%)	1 (0%)	44	76
9	A	565/575 (98%)	465 (82%)	99 (18%)	1 (0%)	44	76
10	H	193/202 (96%)	147 (76%)	46 (24%)	0	100	100
11	L	183/203 (90%)	145 (79%)	35 (19%)	3 (2%)	8	38
12	M	165/212 (78%)	122 (74%)	41 (25%)	2 (1%)	11	43
13	N	206/228 (90%)	160 (78%)	46 (22%)	0	100	100
All	All	5001/6262 (80%)	4015 (80%)	962 (19%)	24 (0%)	27	61

5 of 24 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	2	611	VAL
1	2	644	VAL
1	2	738	PRO
1	2	740	THR
1	2	575	ASP

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	2	534/781 (68%)	494 (92%)	40 (8%)	11	33
2	3	537/699 (77%)	503 (94%)	34 (6%)	15	38
3	4	562/759 (74%)	530 (94%)	32 (6%)	17	41

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
4	5	535/630 (85%)	483 (90%)	52 (10%)	6	24
5	6	551/718 (77%)	521 (95%)	30 (5%)	18	42
6	7	544/630 (86%)	512 (94%)	32 (6%)	16	40
9	A	494/501 (99%)	472 (96%)	22 (4%)	23	46
10	H	170/176 (97%)	160 (94%)	10 (6%)	16	40
11	L	170/184 (92%)	158 (93%)	12 (7%)	12	35
12	M	149/188 (79%)	141 (95%)	8 (5%)	18	42
13	N	187/205 (91%)	177 (95%)	10 (5%)	19	43
All	All	4433/5471 (81%)	4151 (94%)	282 (6%)	17	37

5 of 282 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
9	A	289	LEU
9	A	514	CYS
11	L	120	ILE
3	4	638	LEU
3	4	600	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 95 such sidechains are listed below:

Mol	Chain	Res	Type
6	7	193	GLN
9	A	273	ASN
6	7	243	GLN
6	7	506	GLN
9	A	508	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

6 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
15	ADP	4	901	-	24,29,29	0.90	1 (4%)	29,45,45	1.63	5 (17%)
14	ATP	2	901	-	26,33,33	0.88	1 (3%)	31,52,52	1.69	7 (22%)
15	ADP	6	901	-	24,29,29	0.91	1 (4%)	29,45,45	1.53	3 (10%)
14	ATP	3	901	-	26,33,33	0.94	1 (3%)	31,52,52	1.73	5 (16%)
14	ATP	5	801	-	26,33,33	0.93	1 (3%)	31,52,52	1.72	8 (25%)
15	ADP	7	801	-	24,29,29	0.93	1 (4%)	29,45,45	1.55	5 (17%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
15	ADP	4	901	-	-	5/12/32/32	0/3/3/3
14	ATP	2	901	-	-	7/18/38/38	0/3/3/3
15	ADP	6	901	-	-	4/12/32/32	0/3/3/3
14	ATP	3	901	-	-	5/18/38/38	0/3/3/3
14	ATP	5	801	-	-	3/18/38/38	0/3/3/3
15	ADP	7	801	-	-	0/12/32/32	0/3/3/3

The worst 5 of 6 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	7	801	ADP	C5-C4	2.55	1.47	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	3	901	ATP	C5-C4	2.46	1.47	1.40
14	5	801	ATP	C5-C4	2.44	1.47	1.40
15	6	901	ADP	C5-C4	2.30	1.47	1.40
15	4	901	ADP	C5-C4	2.26	1.46	1.40

The worst 5 of 33 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
15	4	901	ADP	PA-O3A-PB	-5.09	115.34	132.83
14	2	901	ATP	PA-O3A-PB	-4.51	117.36	132.83
14	5	801	ATP	PA-O3A-PB	-4.50	117.38	132.83
15	6	901	ADP	PA-O3A-PB	-4.44	117.58	132.83
14	3	901	ATP	PB-O3B-PG	-4.38	117.79	132.83

There are no chirality outliers.

5 of 24 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
14	2	901	ATP	C5'-O5'-PA-O1A
14	2	901	ATP	C5'-O5'-PA-O2A
14	3	901	ATP	C5'-O5'-PA-O1A
14	3	901	ATP	C5'-O5'-PA-O2A
15	6	901	ADP	C5'-O5'-PA-O3A

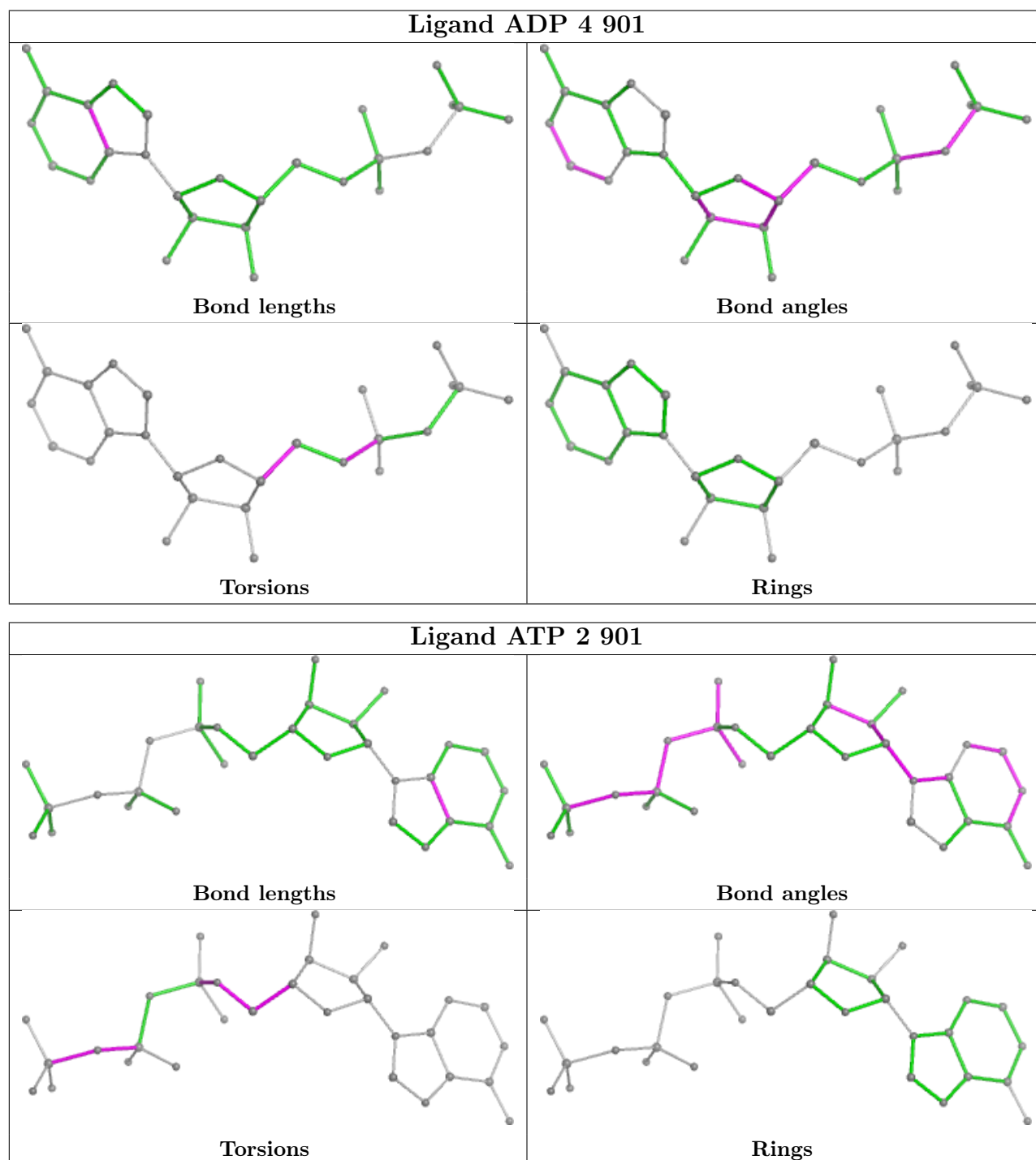
There are no ring outliers.

6 monomers are involved in 30 short contacts:

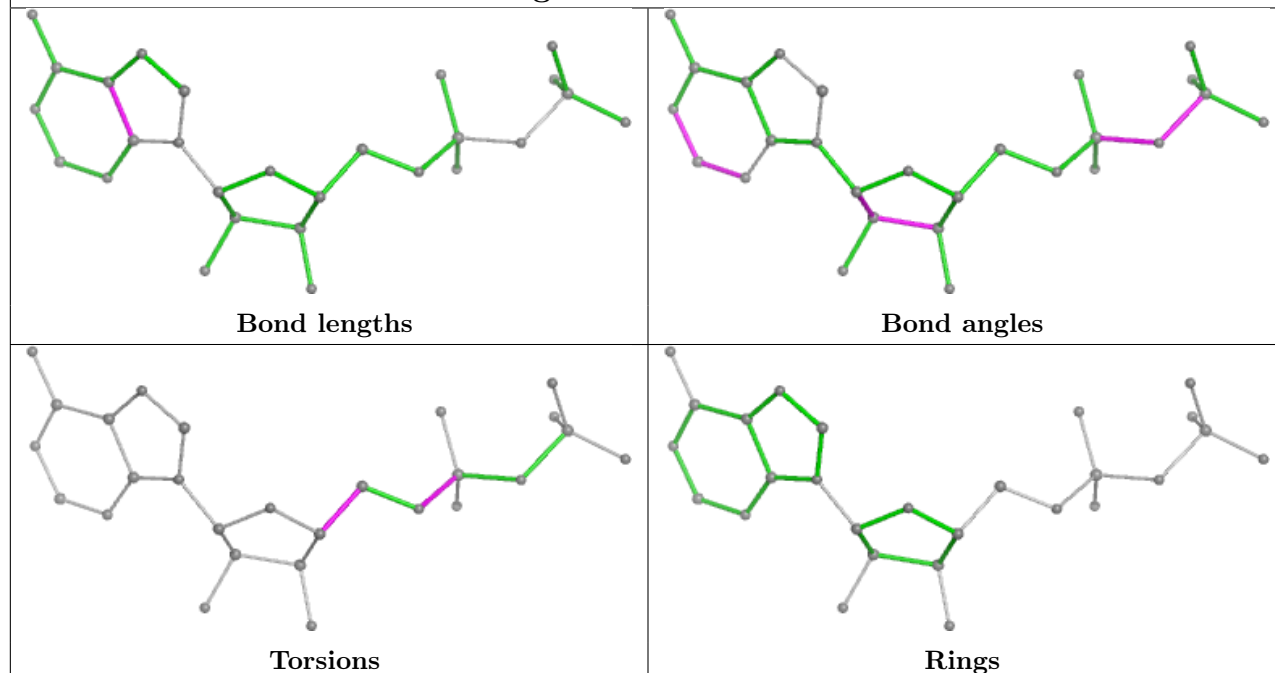
Mol	Chain	Res	Type	Clashes	Symm-Clashes
15	4	901	ADP	2	0
14	2	901	ATP	2	0
15	6	901	ADP	3	0
14	3	901	ATP	10	0
14	5	801	ATP	5	0
15	7	801	ADP	8	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be

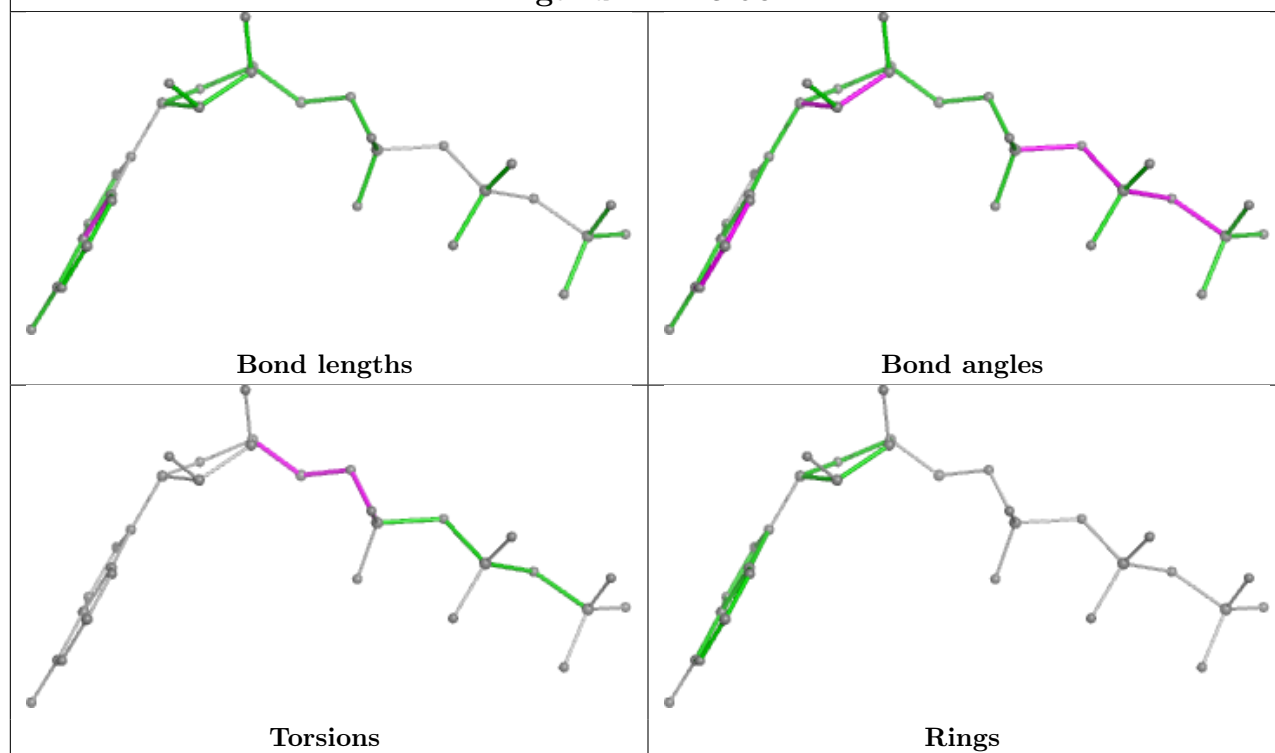
highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

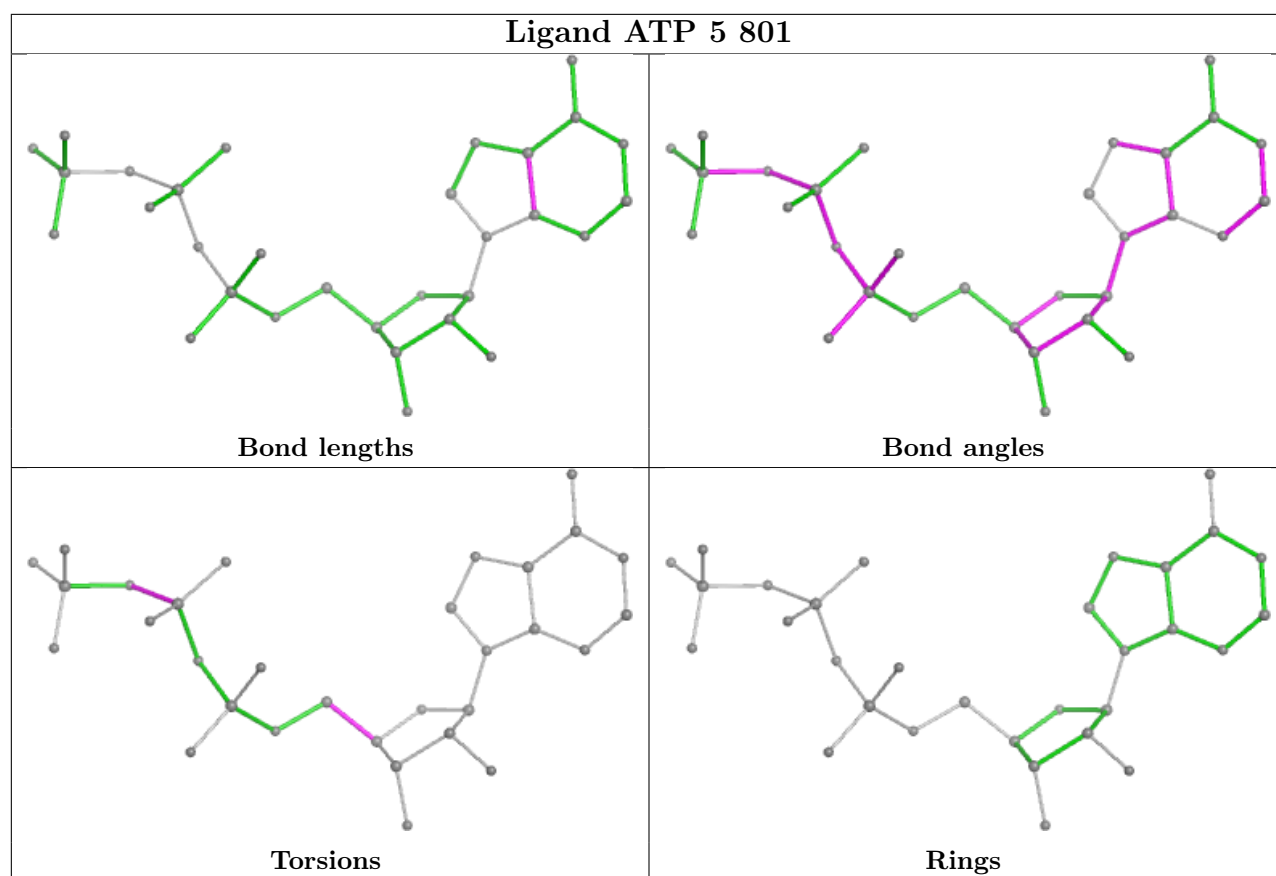


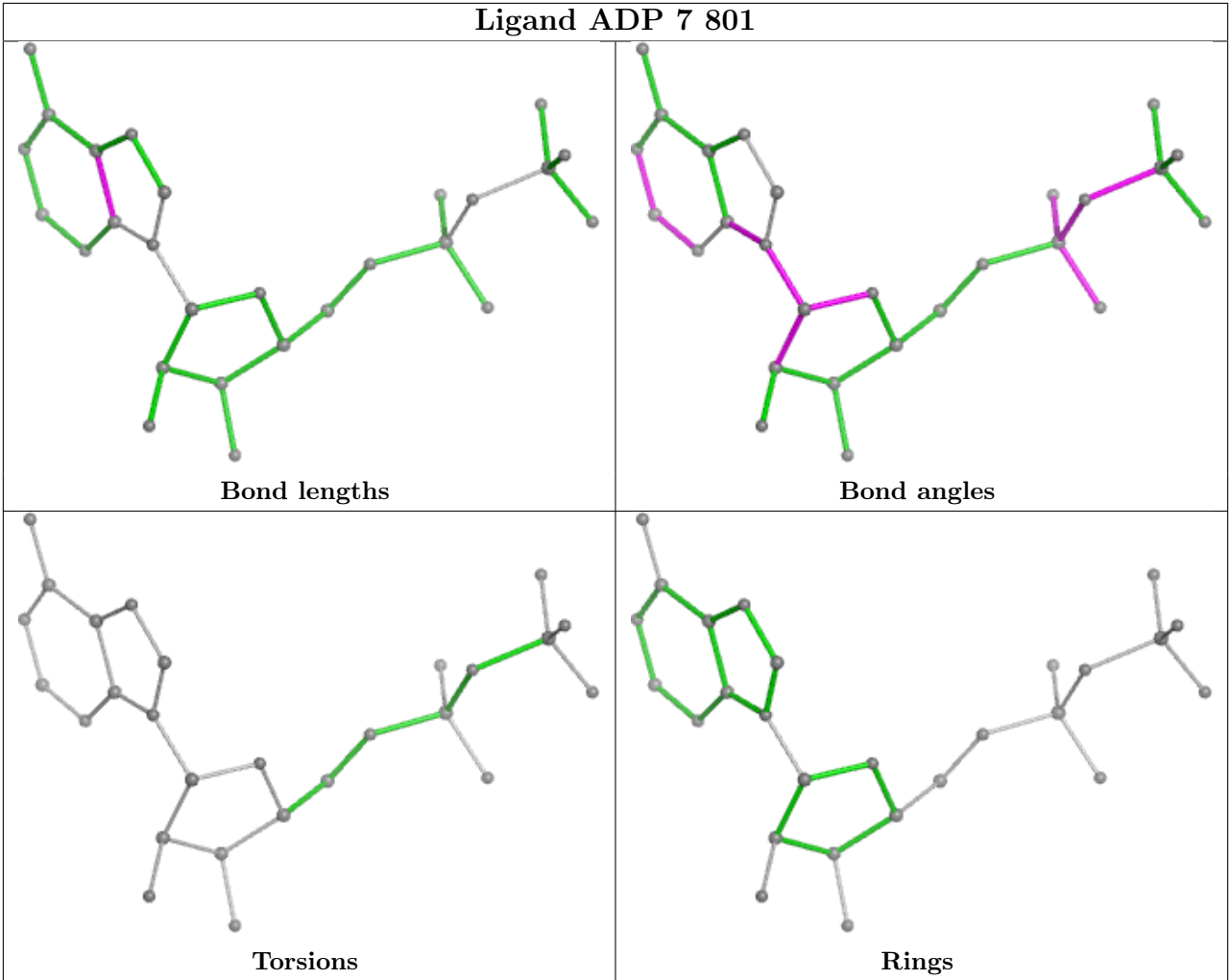
Ligand ADP 6 901



Ligand ATP 3 901







5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

The following chains have linkage breaks:

Mol	Chain	Number of breaks
6	7	2
4	5	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	7	316:ASP	C	317:ALA	N	11.10
1	5	405:GLY	C	408:SER	N	5.76

Continued on next page...

Continued from previous page...

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	7	142:SER	C	143:THR	N	5.51

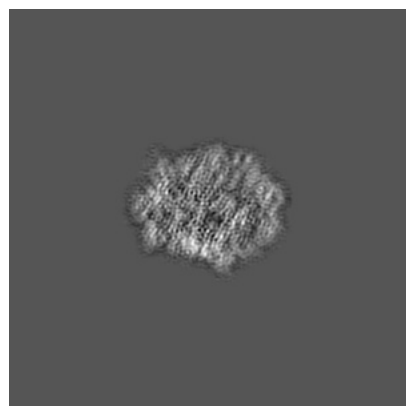
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-4786. These allow visual inspection of the internal detail of the map and identification of artifacts.

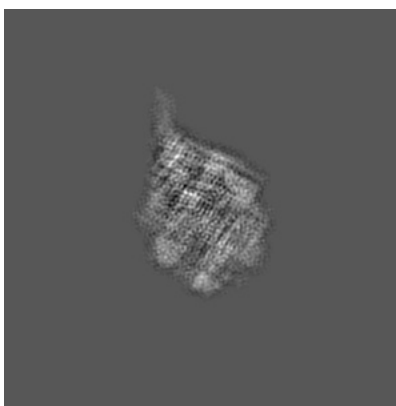
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

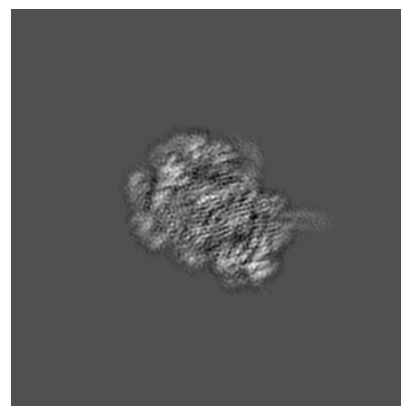
6.1.1 Primary map



X

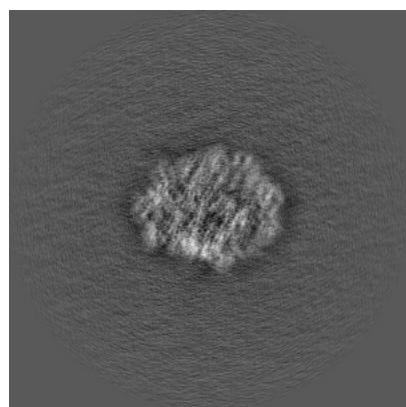


Y

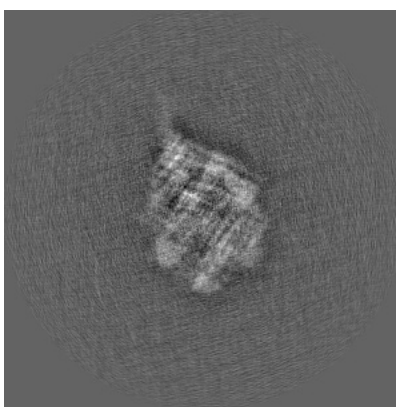


Z

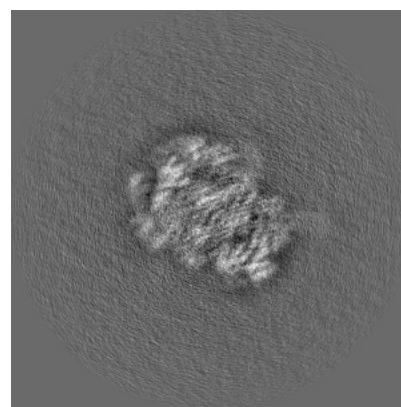
6.1.2 Raw map



X



Y

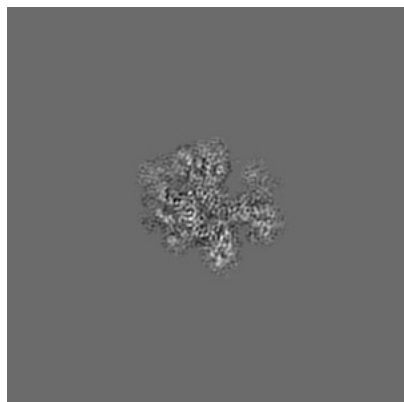


Z

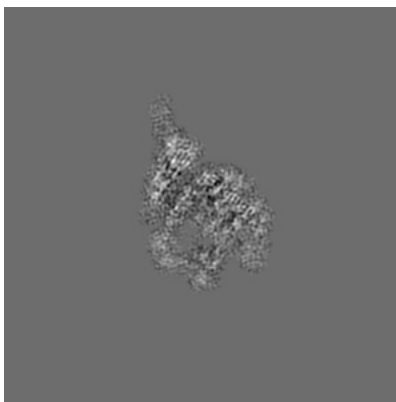
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

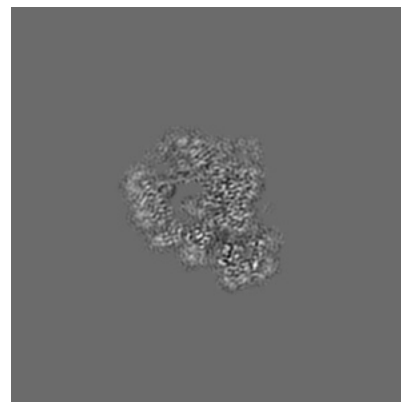
6.2.1 Primary map



X Index: 192

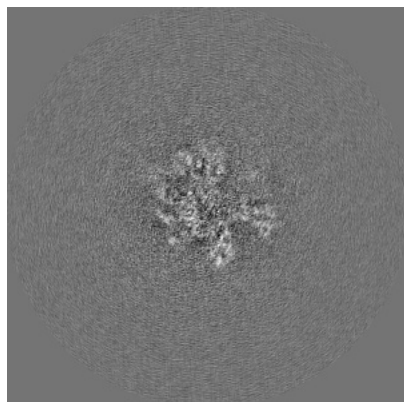


Y Index: 192

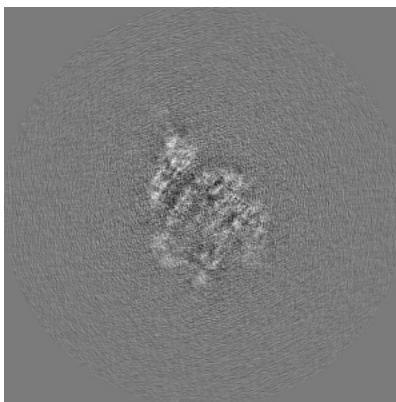


Z Index: 192

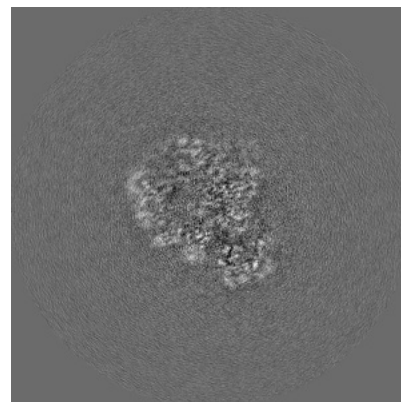
6.2.2 Raw map



X Index: 192



Y Index: 192

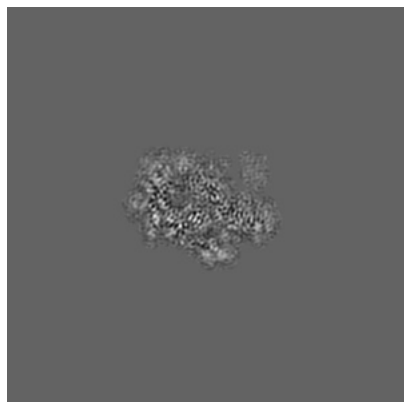


Z Index: 192

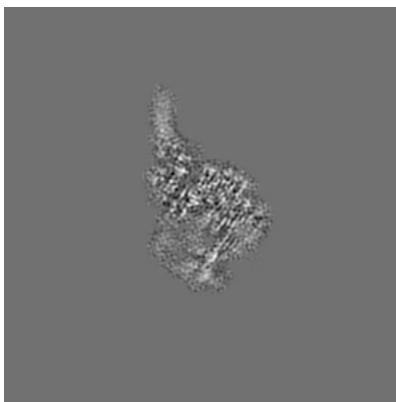
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

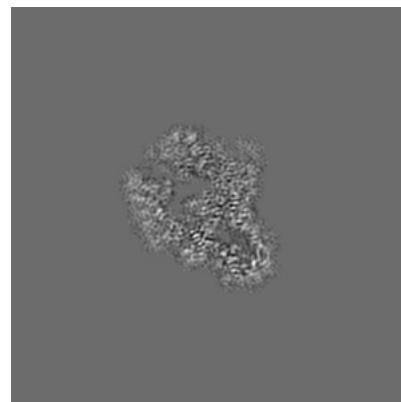
6.3.1 Primary map



X Index: 205

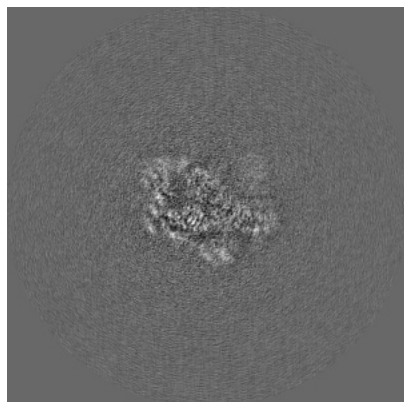


Y Index: 185

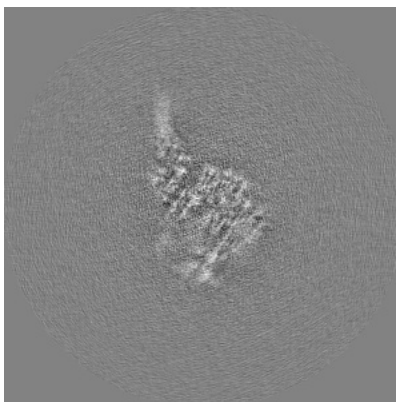


Z Index: 197

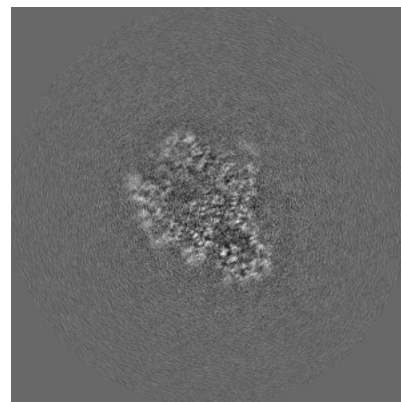
6.3.2 Raw map



X Index: 202



Y Index: 185

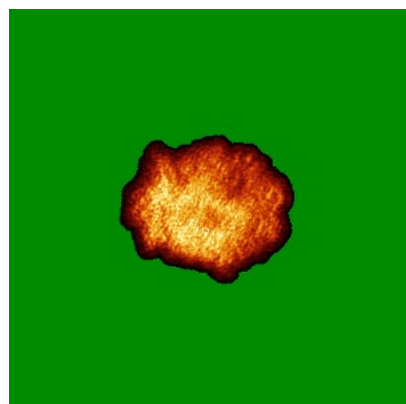


Z Index: 196

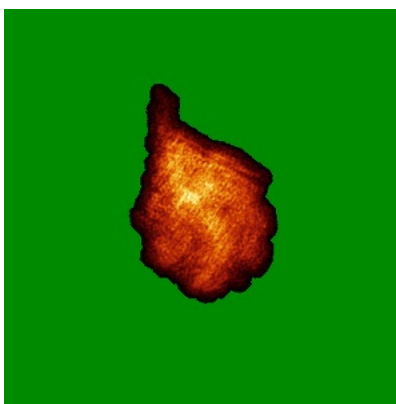
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal standard-deviation projections (False-color) [i](#)

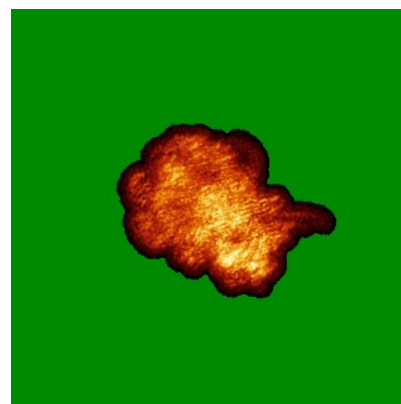
6.4.1 Primary map



X

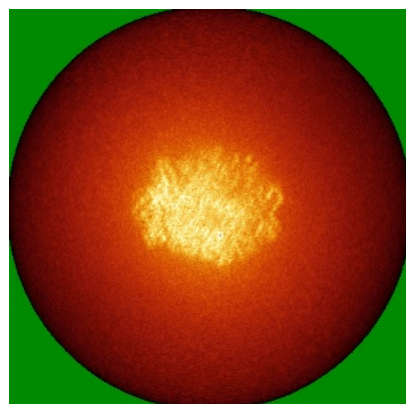


Y

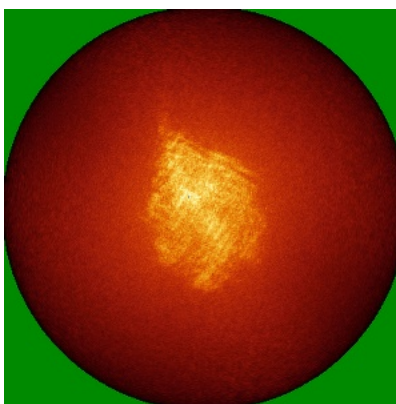


Z

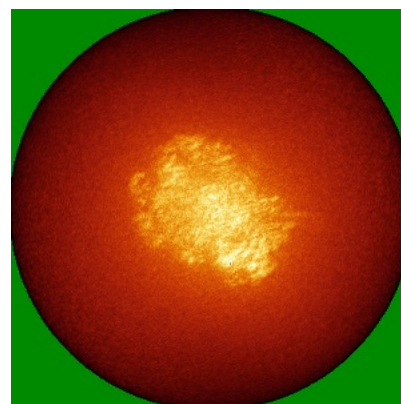
6.4.2 Raw map



X



Y



Z

The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

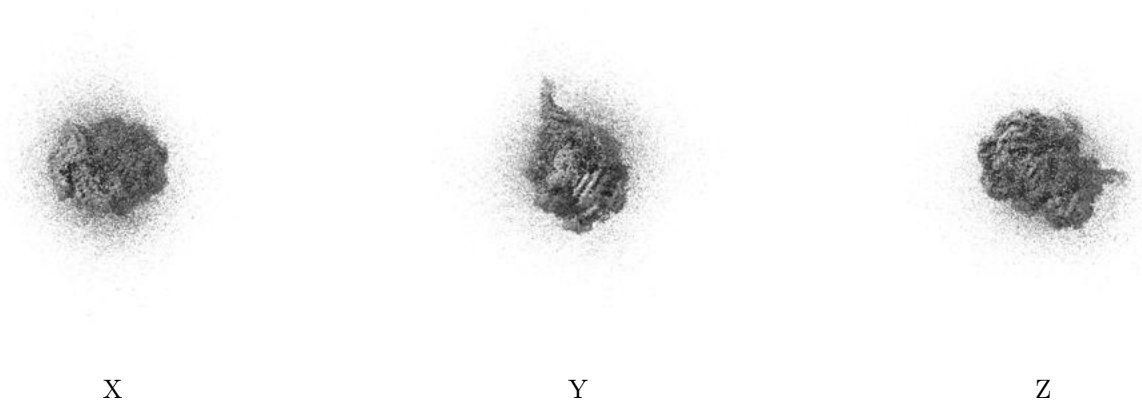
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.006. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



These images show the 3D surface of the raw map. The raw map's contour level was selected so that its surface encloses the same volume as the primary map does at its recommended contour level.

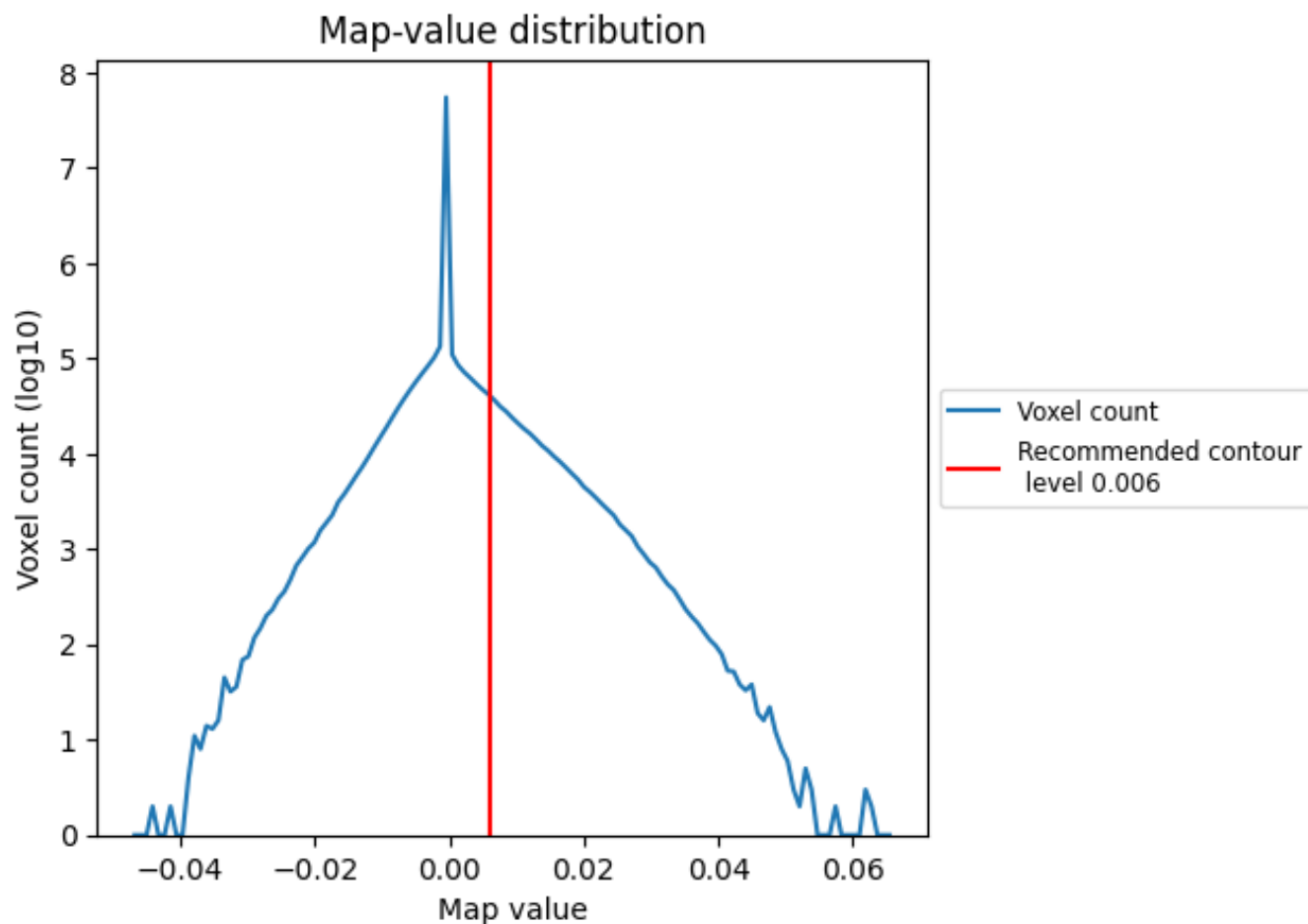
6.6 Mask visualisation [i](#)

This section was not generated. No masks/segmentation were deposited.

7 Map analysis [i](#)

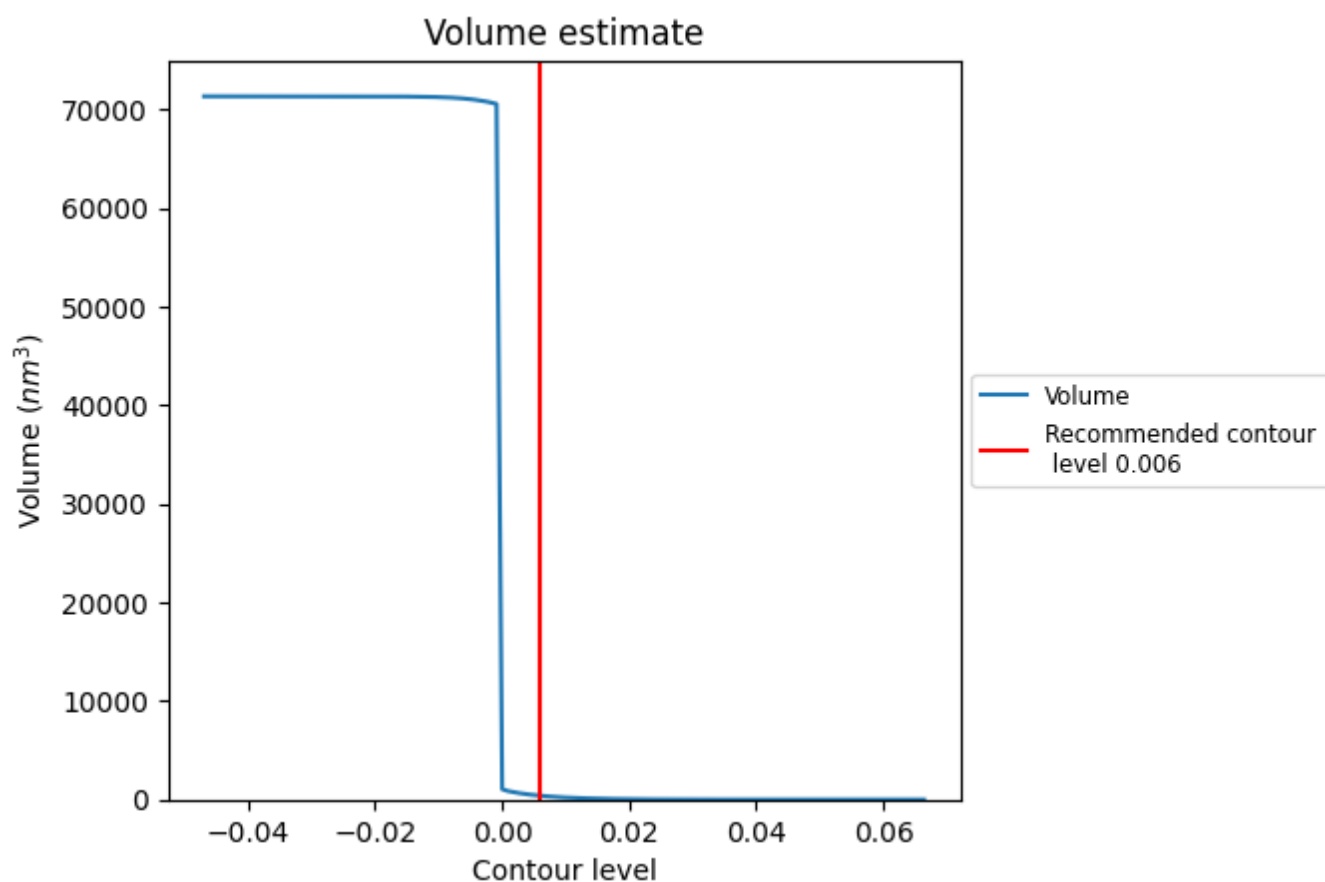
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.

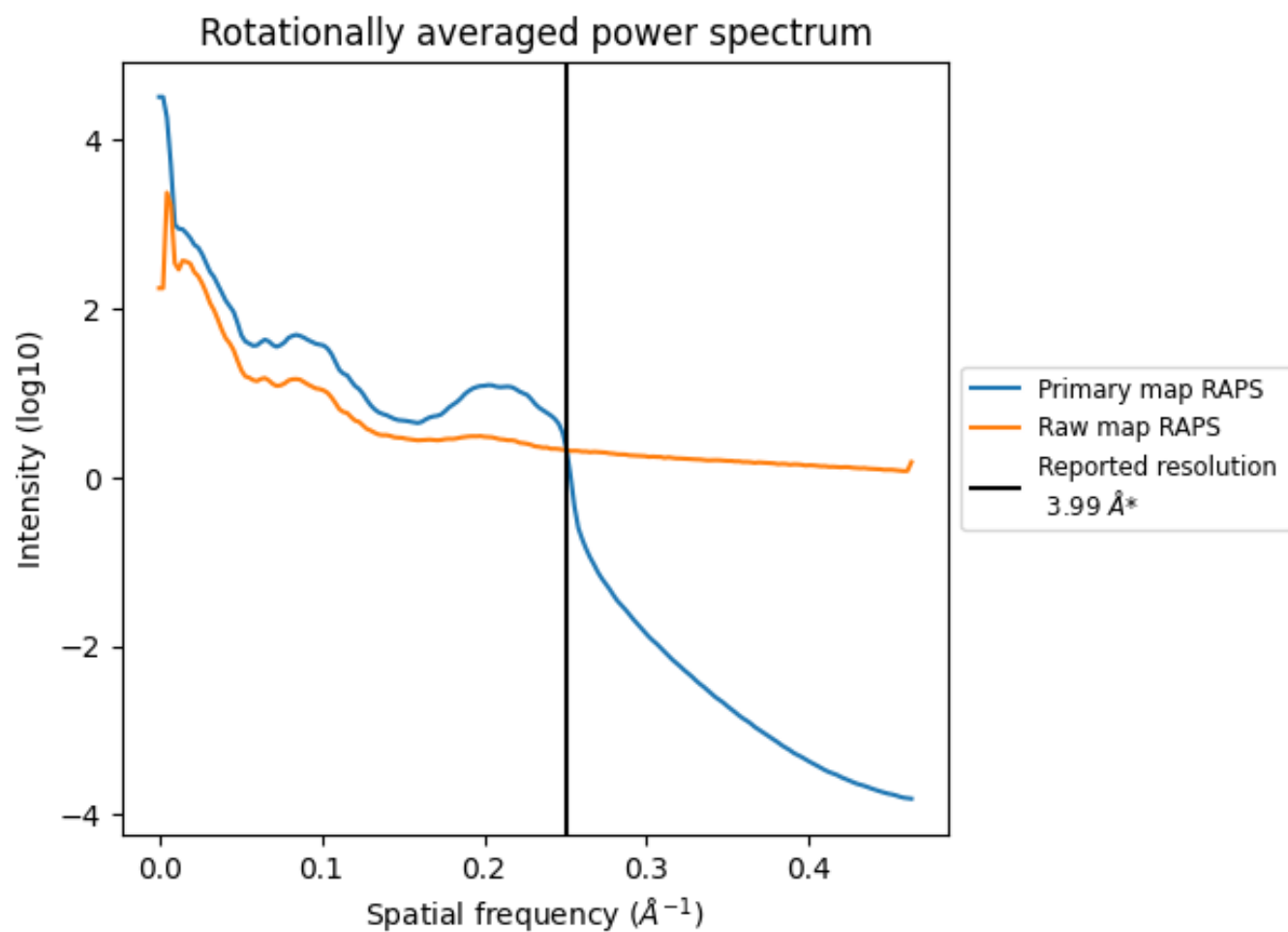
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 393 nm³; this corresponds to an approximate mass of 355 kDa.

The volume estimate graph shows how the enclosed volume varies with the contour level. The recommended contour level is shown as a vertical line and the intersection between the line and the curve gives the volume of the enclosed surface at the given level.

7.3 Rotationally averaged power spectrum ⓘ

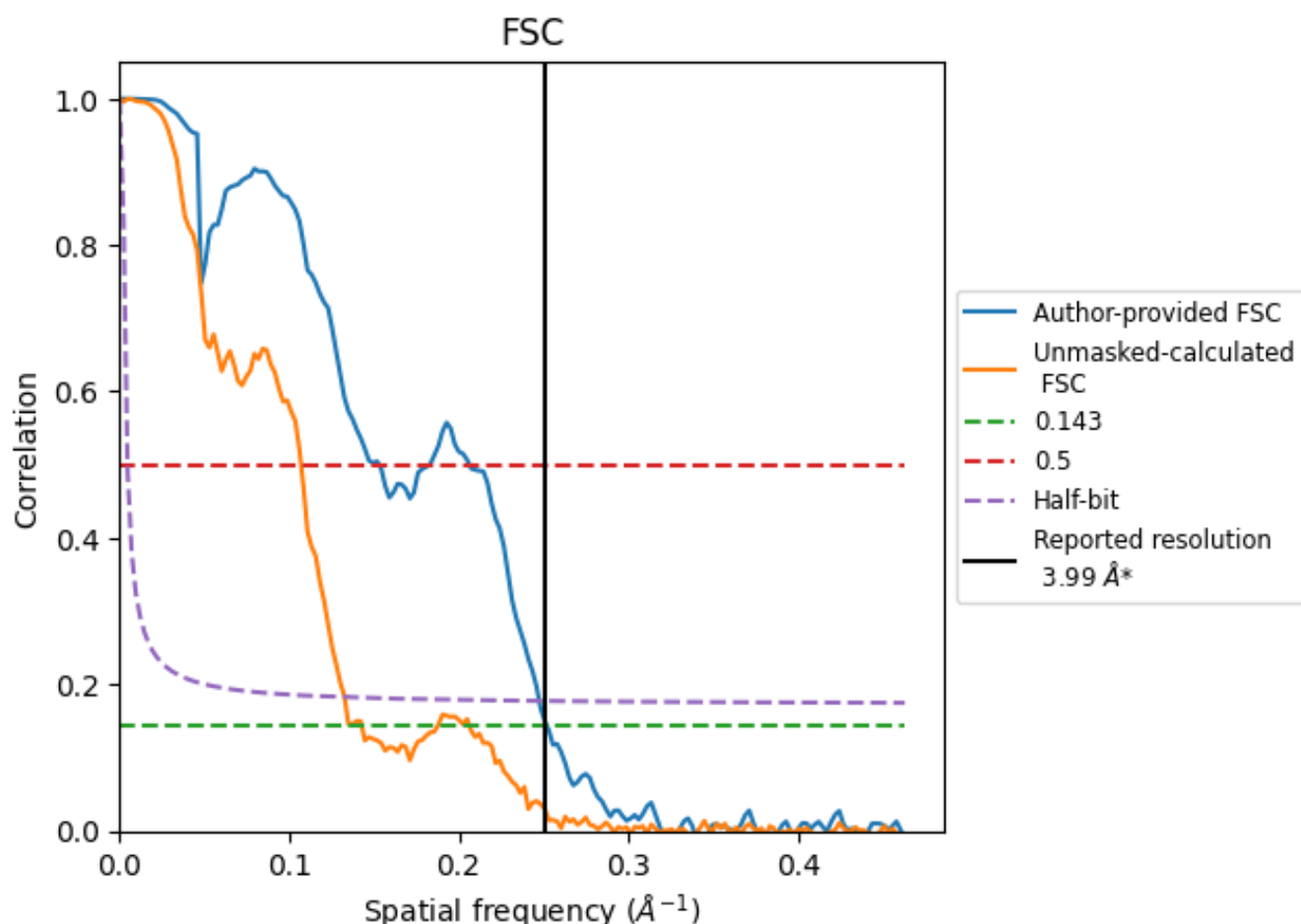


*Reported resolution corresponds to spatial frequency of 0.251 Å⁻¹

8 Fourier-Shell correlation [i](#)

Fourier-Shell Correlation (FSC) is the most commonly used method to estimate the resolution of single-particle and subtomogram-averaged maps. The shape of the curve depends on the imposed symmetry, mask and whether or not the two 3D reconstructions used were processed from a common reference. The reported resolution is shown as a black line. A curve is displayed for the half-bit criterion in addition to lines showing the 0.143 gold standard cut-off and 0.5 cut-off.

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.251 \AA^{-1}

8.2 Resolution estimates [i](#)

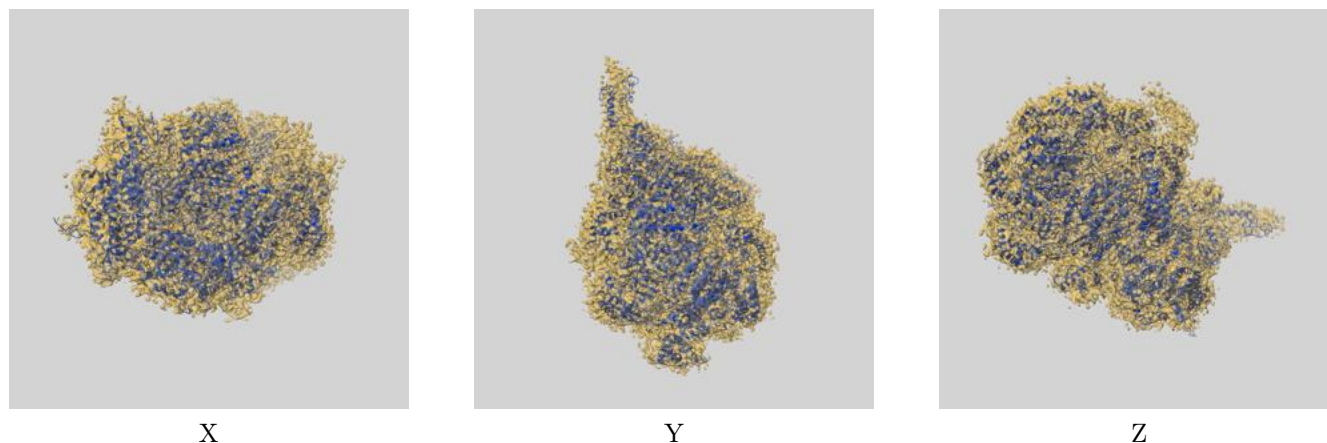
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.99	-	-
Author-provided FSC curve	3.97	6.54	4.04
Unmasked-calculated*	7.00	9.34	7.54

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 7.00 differs from the reported value 3.99 by more than 10 %

9 Map-model fit [i](#)

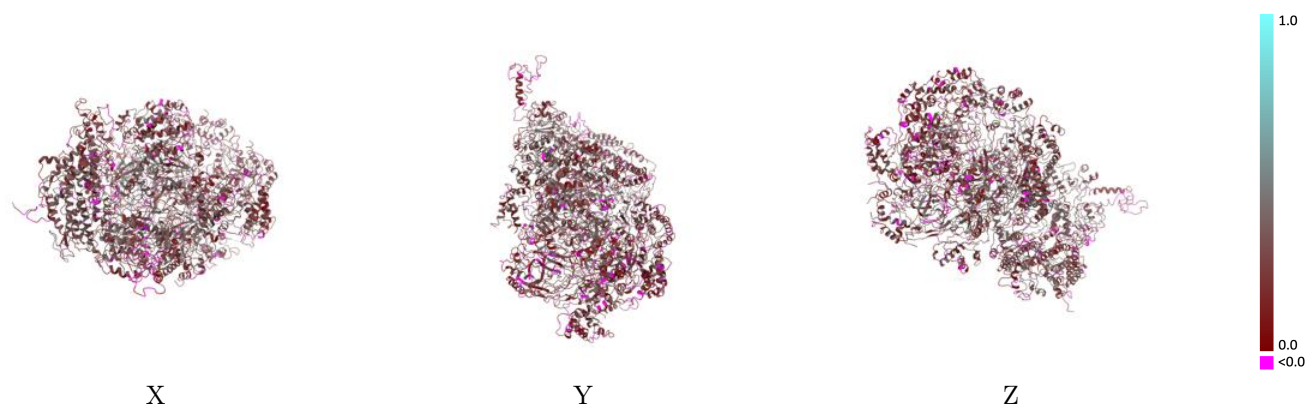
This section contains information regarding the fit between EMDB map EMD-4786 and PDB model 6RAX. Per-residue inclusion information can be found in [section 3](#) on [page 8](#).

9.1 Map-model overlay [i](#)



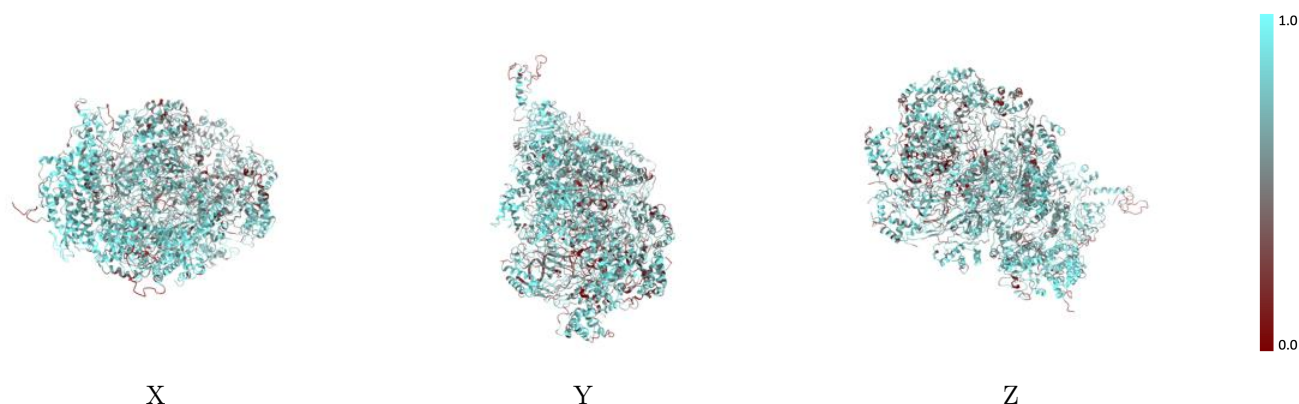
The images above show the 3D surface view of the map at the recommended contour level 0.006 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

9.2 Q-score mapped to coordinate model [i](#)



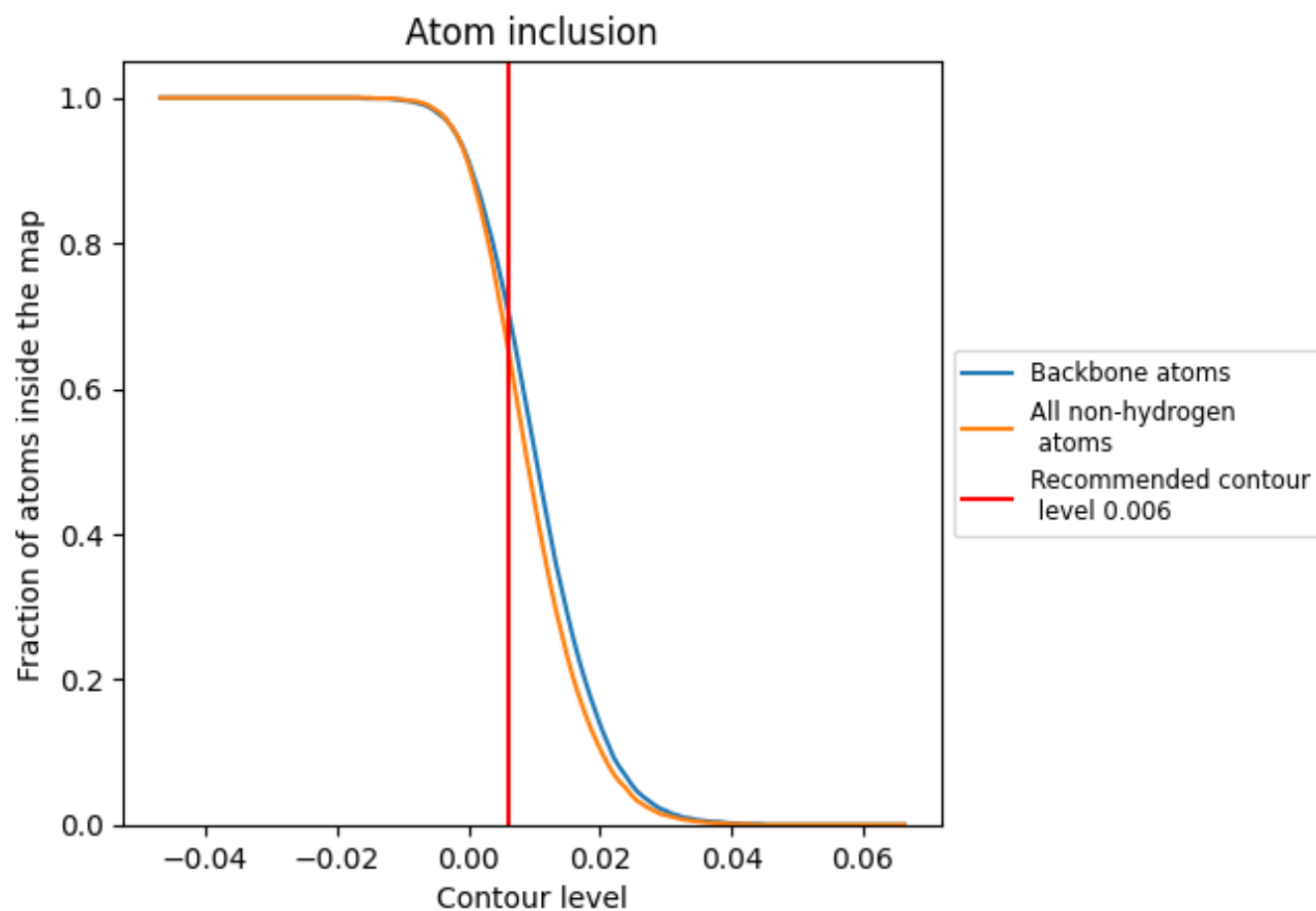
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions at which atoms can be resolved. Low Q-score values may therefore be expected for many entries.

9.3 Atom inclusion mapped to coordinate model [i](#)



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.006).





























9.4 Atom inclusion [i](#)



At the recommended contour level, 71% of all backbone atoms, 66% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary

The table lists the average atom inclusion at the recommended contour level (0.006) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.6580	 0.2550
2	 0.6820	 0.2740
3	 0.6620	 0.2570
4	 0.6000	 0.2010
5	 0.6880	 0.3080
6	 0.6190	 0.2340
7	 0.6070	 0.2310
A	 0.7190	 0.2900
H	 0.6500	 0.2090
L	 0.7840	 0.3110
M	 0.6790	 0.2560
N	 0.7460	 0.2750
X	 0.3920	 0.1550
Y	 0.3230	 0.0660

